

Toluene

108-88-3 | DTXSID7021360

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 3.42 days

Global applicability domain: Inside

Local applicability domain index: 7.62e-01

Confidence level: 7.66e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Toluene</div> <div>Measured: 4.93</div> <div>Predicted: 3.42</div>	<div>Image not found</div> <div>Methylcyclohexane</div> <div>Measured: 24.3</div> <div>Predicted: 4.12</div>	<div>Image not found</div> <div>1,2,4-Trimethylbenzene</div> <div>Measured: 24.3</div> <div>Predicted: 4.83</div>
<div>Image not found</div> <div>para-Xylene</div> <div>Measured: 157</div> <div>Predicted: 5.33</div>	<div>Image not found</div> <div>m-Xylene</div> <div>Measured: 201</div> <div>Predicted: 9.25</div>	